Exact path integral of the hydrogen atom and the Jacobi's principle of least action*

Kazuo Fujikawa
Department of Physics, University of Tokyo
Bunkyo-ku, Tokyo 113, Japan

The general treatment of a separable Hamiltonian of Liouville-type is well-known in operator formalism. A path integral counterpart is formulated if one starts with the Jacobi's principle of least action, and a path integral evaluation of the Green's function for the hydrogen atom by Duru and Kleinert is recognized as a special case. The Jacobi's principle of least action for given energy is reparametrization invariant, and the separation of variables in operator formalism corresponds to a choice of gauge in path integral. The Green's function is shown to be gauge independent,if the operator ordering is properly taken into account. These properties are illustrated by evaluating an exact path integral of the Green's function for the hydrogen atom in parabolic coordinates.

I. INTRODUCTION

The path integral treatment of the hydrogen atom is interesting not only for a methodological interest but also for a pedagogical purpose. After several early attempts[1,2], Duru and Kleinert[3] showed an elegant path integral method to evaluate the Green's function for the hydrogen atom exactly. Two basic ingredients in their method are the use of a re-scaled time variable and the so called Kustaanheimo-Stiefel transformation[4]which reveals the O(4) symmetry explicitly in the coordinate space. Many of the clarifying works of this approach have been published [5] - [14]. It has been shown elsewhere[15] that this problem is treated in a more general setting of gauge theory if one formulates the problem on the basis of the Jacobi's principle of least action, which is reparametrization invariant.

The general technique of gauge theory is thus applicable to the evaluation of path integral, and a suitable choice of gauge simplifies the problem such as the hydrogen atom. In particular, the Green's function is shown to be gauge independent. The use of the Kustaanheimo-Stiefel transformation is rather technical and it is not essential in solving the problem exactly. We in fact show a simple trick in parabolic coordinates[16] which solves the hydrogen atom exactly.

II. HYDROGEN ATOM

2.1, Analysis in Parabolic Coordinates

We analyze the hydrogen atom by starting with the Hamiltonian written in terms of parabolic coordinates

$$H(\xi,\eta,\varphi)=\frac{1}{2m(\xi+\eta)}(\xi p_\xi^2+\eta p_\eta^2)+\frac{1}{8m\xi\eta}p_\varphi^2-\frac{e^2}{\xi+\eta} \tag{1}$$

where the parabolic coordinates are introduced by $\xi=\frac{1}{2}(r-z),\eta=\frac{1}{2}(r+z)$ and φ stands for the azimuthal angle around the z axis. We further perform a canonical transformation which simplifies the kinetic term in H as

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$$\begin{aligned}
\xi &= \frac{1}{4}u^2 \qquad , 0 \le u < \infty \\
\sqrt{\xi} p_\xi &= p_u \\
\eta &= \frac{1}{4}v^2 \qquad , 0 \le v < \infty \\
\sqrt{\eta} p_\eta &= p_v
\end{aligned} \tag{2}$$

and the Hamiltonian becomes

$$H = \frac{1}{2m}(\frac{4}{u^2+v^2})[p_u^2 + \frac{1}{u^2}p_\varphi^2 + p_v^2 + \frac{1}{v^2}p_\varphi^2] - \frac{4}{u^2+v^2}e^2 \tag{3}$$

where $r = \xi + \eta = (u^2+v^2)/4$. This Hamiltonian is not yet a separable one of Liouville-type.

One may solve the Schroedinger equation

$$\hat{H}\psi = E\psi \tag{4}$$

or equivalently

$$\hat{H}_T\psi = 0 \tag{5}$$

with

$$\hat{H}_T = \frac{1}{2m}[\hat{p}_u^2 + \frac{1}{u^2}\hat{p}_\varphi^2 + \hat{p}_v^2 + \frac{1}{v^2}\hat{p}_\varphi^2] - e^2 + \frac{m\omega^2}{2}(u^2+v^2) \tag{6}$$

where ω is defined by

$$\frac{1}{2}m\omega^2 = -\frac{1}{4}E \tag{7}$$

We consider the case $E < 0$ for the moment. $\hat{H}_T$ stands for the total Hamiltonian defined by a specific gauge condition; a general definition of $\hat{H}_T$ will be given later in (39).

Eq.(5) may be rewritten in an equivalent form as

$$\begin{aligned}
\hat{\tilde{H}}_T\psi &= 0 \\
(\hat{p}_\varphi - \hat{p}_{\varphi'})\psi &= 0
\end{aligned} \tag{8}$$

We here introduced auxiliary variables $(\hat{p}_{\varphi'}, \varphi')$ as

$$\begin{aligned}
\hat{\tilde{H}}_T &= \frac{1}{2m}[\hat{p}_u^2 + \frac{1}{u^2}\hat{p}_\varphi^2 + \hat{p}_v^2 + \frac{1}{v^2}\hat{p}_{\varphi'}] + \frac{m\omega^2}{2}(u^2+v^2) - e^2 \\
&= \frac{1}{2m}\vec{p}_u^{\,2} + \frac{m\omega^2}{2}\vec{u}^2 + \frac{1}{2m}\vec{p}_v^{\,2} + \frac{m\omega^2}{2}\vec{v}^2 - e^2
\end{aligned} \tag{9}$$

and we defined

$$\begin{aligned}
\vec{u} &= (u_1, u_2) = (u\cos\varphi, u\sin\varphi) \\
\vec{p}_u^{\,2} &= \hat{p}_u^2 + \frac{1}{u^2}\hat{p}_\varphi^2 \\
\vec{v} &= (v_1, v_2) = (v\cos\varphi', v\sin\varphi') \\
\vec{p}_v^{\,2} &= \hat{p}_v^2 + \frac{1}{v^2}\hat{p}_{\varphi'}^2
\end{aligned} \tag{10}$$

The subsidiary condition in (8) replaces the use of the Kustaanheimo-Stiefel transformation, and at the same time it renders a Hamiltonian of Liouville-type. This introduction of auxiliary variables (10) has been discussed by Ravndal and Toyoda[16].

A general procedure to deal with a completely separated operator such as $\hat{\tilde{H}}_T$ in (9) is to consider an evolution operator for a parameter τ defined by

$$\begin{aligned}
&\langle \vec{u}_b, \vec{v}_b | e^{-i\hat{\tilde{H}}_T \tau/\hbar} | \vec{u}_a, \vec{v}_a \rangle \\
&= e^{ie^2\tau} \langle \vec{u}_b | exp[-(i/\hbar)(\frac{1}{2m}\vec{p}_u^{\,2} + \frac{m\omega^2}{2}\vec{u}^2)\tau] | \vec{u}_a \rangle \\
&\times \langle \vec{v}_b | exp[-(i/\hbar)(\frac{1}{2m}\vec{p}_v^{\,2} + \frac{m\omega^2}{2}\vec{v}^2)\tau] | \vec{v}_a \rangle \\
&= e^{ie^2\tau} (\frac{m\omega}{2\pi i\hbar \sin\omega\tau})^{4/2} \\
&\times exp\{\frac{im\omega}{2\hbar \sin\omega\tau}[(\vec{u}_b^{\,2} + \vec{v}_b^{\,2} + \vec{u}_a^{\,2} + \vec{v}_a^{\,2})\cos\omega\tau - 2\vec{u}_b\vec{u}_a - 2\vec{v}_b\vec{v}_a]\}
\end{aligned} \tag{11}$$

where we used the exact result for a simple harmonic oscillator[17].

A crucial observation here is that $\hat{p}_\varphi$ and $\hat{p}_{\varphi'}$ are preserved during the evolution dictated by the operator $\hat{\tilde{H}}_T$ in (9), since $[\hat{p}_\varphi, \hat{\tilde{H}}_T] = [\hat{p}_{\varphi'}, \hat{\tilde{H}}_T] = 0$. It is then sufficient to impose the constraint (8) only on the initial state , for example. Starting with a general state belonging to the eigenvalues $\hat{p}_\varphi = m$ and $\hat{p}_{\varphi'} = m'$

$$e^{im\varphi} e^{im'\varphi'} \tag{12}$$

we can use the following trick

$$\int_0^{2\pi} \frac{d\theta}{2\pi} e^{im(\varphi+\theta)} e^{im'(\varphi'-\theta)} = \delta_{m,m'} e^{im(\varphi+\varphi')} \tag{13}$$

to project out the state satisfying $\hat{p}_\varphi = \hat{p}_{\varphi'}$, and $\varphi + \varphi'$ is regarded as the actual azimuthal angle.

We thus obtain

$$\begin{aligned}
&\langle u_b, v_b, (\varphi+\varphi')_b | e^{-i\hat{H}_T \tau/\hbar} | u_a, v_a, (\varphi+\varphi')_a \rangle \\
&= e^{ie^2\tau} (\frac{m\omega}{2\pi i\hbar \sin\omega\tau})^2 \int_0^{2\pi} \frac{d\theta}{2\pi} exp\{\frac{im\omega}{2\hbar \sin\omega\tau}[(\vec{u}_b^{\,2} + \vec{v}_b^{\,2} + \vec{u}_a^{\,2} + \vec{v}_a^{\,2})\cos\omega\tau - 2\vec{u}_b\vec{u}_a - 2\vec{v}_b\vec{v}_a]\} \\
&= e^{ie^2\tau} (\frac{m\omega}{2\pi i\hbar \sin\omega\tau})^2 \times \\
&\int_0^{2\pi} \frac{d\theta}{2\pi} exp\{\frac{im\omega}{2\hbar \sin\omega\tau}[4(\xi_a + \xi_b + \eta_a + \eta_b)\cos\omega\tau - 4\sqrt{2}(r_a r_b + \vec{x}_a\vec{x}_b)^{1/2}\cos(\theta+\gamma)]\} \\
&= e^{ie^2\tau} (\frac{m\omega}{2\pi i\hbar \sin\omega\tau})^2 exp\{\frac{2im\omega}{\hbar \sin\omega\tau}(r_a + r_b)\cos\omega\tau\} I_0(\frac{2\sqrt{2}im\omega}{\hbar \sin\omega\tau}(r_a r_b + \vec{x}_a\vec{x}_b)^{1/2})
\end{aligned} \tag{14}$$

In this evaluation we start with the relation

$$\vec{u}_b\vec{u}_a + \vec{v}_b\vec{v}_a = u_b u_a \cos\Delta\varphi + v_b v_a \cos\Delta\varphi' \tag{15}$$

with $\Delta\varphi = \varphi_b - \varphi_a, \Delta\varphi' = \varphi'_b - \varphi'_a$, and

$$
\begin{aligned}
&u_b u_a \cos(\Delta\varphi+\theta)+v_b v_a\cos(\Delta\varphi'-\theta)\\
&=(u_b u_a\cos\Delta\varphi+v_b v_a\cos\Delta\varphi')\cos\theta\\
&+(-u_b u_a\sin\Delta\varphi+v_b v_a\sin\Delta\varphi')\sin\theta\\
&=4\sqrt{\xi_b\xi_a+\eta_b\eta_a+2\sqrt{\xi_b\xi_a\eta_b\eta_a}\cos(\Delta\varphi+\Delta\varphi')}\cos(\theta+\gamma)\\
&=2\sqrt{2}\sqrt{r_a r_b+z_a z_b+\rho_a\rho_b\cos(\Delta\varphi+\Delta\varphi')}\cos(\theta+\gamma)\\
&=2\sqrt{2}\sqrt{r_a r_b+\vec{x}_a\vec{x}_b}\cos(\theta+\gamma)
\end{aligned}
\tag{16}
$$

where we used the definition of variables in (2), and γ is a number independent of θ. We also defined a modified Bessel function

$$
I_0(\frac{2\sqrt{2}im\omega}{\hbar\sin\omega\tau}(r_a r_b+\vec{x}_a\vec{x}_b)^{1/2})=\int_0^{2\pi}\frac{d\theta}{2\pi}exp\{\frac{2\sqrt{2}im\omega(r_a r_b+\vec{x}_a\vec{x}_b)^{1/2}}{\hbar\sin\omega\tau}\cos\theta\}
\tag{17}
$$

The parameter τ is arbitrary, and we eliminate τ to obtain a physically meaningful quantity by

$$
\begin{aligned}
&i\int_0^\infty d\tau\langle u_b,v_b,(\varphi+\varphi')_b|e^{-i\hat{H}_T\tau/\hbar}|u_a,v_a,(\varphi+\varphi')_a\rangle\\
&=\langle u_b,v_b,(\varphi+\varphi')_b|\frac{\hbar}{\hat{H}_T}|u_a,v_a,(\varphi+\varphi')_a\rangle\\
&=i\int_0^\infty d\tau e^{ie^2\tau}(\frac{m\omega}{2\pi i\hbar\sin\omega\tau})^2 exp\{\frac{2im\omega}{\hbar\sin\omega\tau}(r_a+r_b)\cos\omega\tau\}\\
&\times I_0(\frac{2\sqrt{2}im\omega}{\hbar\sin\omega\tau}(r_a r_b+\vec{x}_a\vec{x}_b)^{1/2})\\
&=\frac{m\omega}{2\pi^2\hbar^2}\int_0^1 d\lambda\lambda^{-\nu}\frac{1}{(1-\lambda)^2}exp[\frac{-2m\omega}{\hbar}(r_a+r_b)(\frac{1+\lambda}{1-\lambda})]I_0(\frac{4\sqrt{2}m\omega}{\hbar}\frac{\lambda^{1/2}}{1-\lambda}(r_a r_b+\vec{x}_a\vec{x}_b)^{1/2})
\end{aligned}
\tag{18}
$$

where we rotated τ by 90 degrees , $\tau\to -i\tau$, and defined

$$
\begin{aligned}
\lambda&=e^{-2\omega\tau}\\
\nu&=e^2/2\omega
\end{aligned}
\tag{19}
$$

We next show that (18) gives an exact Green's function for the hydrogen atom by noting the sequence

$$
\begin{aligned}
&\langle u_b,v_b,\varphi_b|\frac{\hbar}{\hat{H}_T}|u_a,v_a,\varphi_a\rangle\\
&=\langle\xi_b,\eta_b,\varphi_b|\frac{\hbar}{(\frac{1}{\hat{\xi}+\hat{\eta}})\hat{H}_T(\xi,\eta,\varphi)}|\xi_a,\eta_a,\varphi_a\rangle(\frac{1}{\xi_a+\eta_a})\\
&=\langle\xi_b,\eta_b,\varphi_b|\frac{\hbar}{\hat{H}(\xi,\eta,\varphi)-E}|\xi_a,\eta_a,\varphi_a\rangle(\frac{1}{\xi_a+\eta_a})\\
&=\frac{\hbar}{\hat{H}(\xi_b,\eta_b,\varphi_b)-E}(\frac{1}{\sqrt{\xi_b+\eta_b}}\langle\xi_b,\eta_b,\varphi_b|\xi_a,\eta_a,\varphi_a\rangle\frac{1}{\sqrt{\xi_a+\eta_a}})\\
&=\frac{1}{4\pi}\langle\vec{x}_b|\frac{\hbar}{\hat{\vec{p}}^2/2m-e^2/r-E}|\vec{x}_a\rangle
\end{aligned}
\tag{20}
$$

where we used φ in place of $\varphi+\varphi'$ and the relation $(\hat{A}\hat{B})^{-1}=\hat{B}^{-1}\hat{A}^{-1}$.

The volume element changes in this transition from $\hat{H}_T$ to $\hat{H}$ as

$$\begin{aligned} dV_0 &= 2\pi uvdudvd\varphi \\ \rightarrow dV &= (\xi+\eta)dV_0 = 4\pi\times 2(\xi+\eta)d\xi d\eta d\varphi \\ &= 4\pi\times r^2 drd\cos\theta d\varphi \end{aligned} \tag{21}$$

The bra- and ket- vectors in (20) are normalized in the combination

$$\begin{aligned} \int dV_0|u,v,\varphi\rangle\langle u,v,\varphi| &= 1 \\ \int dV|\xi,\eta,\varphi\rangle\frac{1}{\xi+\eta}\langle\xi,\eta,\varphi| &= 1 \\ \int d^3x|\vec{x}\rangle\langle\vec{x}| &= 1 \end{aligned} \tag{22}$$

and the extra factor of 4π in $dV=4\pi r^2drd\cos\theta d\varphi$ requires the appearance of the factor of $1/4\pi$ in the last expression in (20). The appearance of 2π in dV_0 is an artifact of the variable φ' in (10). This normalization condition of bra- and ket- vectors together with a symmetry in $\vec{x}_a$ and $\vec{x}_b$ justify the identification (20). A more explicit and concrete analysis of eqs.(20)$\sim$ (22) will be given in connection with the Jacobi's principle later.

As for the operator ordering, the momentum operator changes in (20) as

$$\begin{aligned} \hat{p}_u^2+\hat{p}_v^2 &= (\frac{\hbar}{i})^2[\frac{1}{u}\partial_u u\partial_u+\frac{1}{v}\partial_v v\partial_v] \\ &= (\frac{\hbar}{i})^2[\partial_\xi\xi\partial_\xi+\partial_\eta\eta\partial_\eta] \\ &= \hat{p}_\xi\xi\hat{p}_\xi+\hat{p}_\eta\eta\hat{p}_\eta \end{aligned} \tag{23}$$

and

$$(\frac{1}{\xi+\eta})(\hat{p}_\xi\xi\hat{p}_\xi+\hat{p}_\eta\eta\hat{p}_\eta)+\frac{1}{4\xi\eta}\hat{p}_\varphi^2=\hat{\vec{p}}^2 \tag{24}$$

where the right-hand side is written in cartesian coordinates. We note that dV_0 and dV in (21) respectively render $\hat{H}_T$ and $\hat{H}(\xi,\eta,\varphi)$ hermitian.

Combining (18),(20) and (24), we have thus established the exact Green's function including the *operator ordering*

$$\begin{aligned} \langle\vec{x}_b|\frac{\hbar}{\hat{\vec{p}}^2/2m-e^2/r-E}|\vec{x}_a\rangle &= \frac{2m^2\omega}{\pi\hbar^2}\int_0^1 d\lambda\lambda^{-\nu}\frac{1}{(1-\lambda)^2}exp[\frac{-2m\omega}{\hbar}(r_a+r_b)(\frac{1+\lambda}{1-\lambda})] \\ &\times I_0(\frac{4\sqrt{2}m\omega}{\hbar}\frac{\lambda^{1/2}}{1-\lambda}(r_ar_b+\vec{x}_a\vec{x}_b)^{1/2}) \end{aligned} \tag{25}$$

It is known that this formula, which was first derived by Duru and Kleinert[3], is a Fourier transform of Schwinger's momentum space representation[18]. The continuation to the scattering problem with $E>0$ is performed by the replacement

$$\omega\rightarrow(-i)\omega,\quad \nu\rightarrow i\nu \tag{26}$$

in the above formula.

One can understand the spectrum of the hydrogen atom by looking at $\hat{\tilde{H}}_T$ in (9)[16]. If one defines the oscillator variables

$$\begin{aligned} a_k &= \frac{1}{\sqrt{2}}[\sqrt{\frac{m\omega}{\hbar}}u_k + \frac{i}{\sqrt{m\omega\hbar}}\hat{p}_{u_k}], \\ \tilde{a}_k &= \frac{1}{\sqrt{2}}[\sqrt{\frac{m\omega}{\hbar}}v_k + \frac{i}{\sqrt{m\omega\hbar}}\hat{p}_{v_k}], \quad k = 1, 2 \end{aligned} \tag{27}$$

one obtains

$$\begin{aligned} \hat{\tilde{H}}_T &= \hbar\omega[\sum_{k=1}^{2}(a_k^\dagger a_k + \tilde{a}_k^\dagger \tilde{a}_k) + 2] - e^2 \\ \hat{p}_\varphi &= i\hbar[a_1^\dagger a_2 - a_2^\dagger a_1] \\ \hat{p}_{\varphi'} &= i\hbar[\tilde{a}_1^\dagger \tilde{a}_2 - \tilde{a}_2^\dagger \tilde{a}_1] \end{aligned} \tag{28}$$

After a unitary transformation

$$\begin{aligned} a_1 &= \frac{1}{\sqrt{2}}(b_1 - ib_2) \\ a_2 &= \frac{1}{\sqrt{2}}(-ib_1 + b_2) \end{aligned} \tag{29}$$

and a similar transformation of $\tilde{a}_1$ and $\tilde{a}_2$, one obtains

$$\begin{aligned} \hat{\tilde{H}}_T &= \hbar\omega[\sum_{k=1}^{2}(b_k^\dagger b_k + \tilde{b}_k^\dagger \tilde{b}_k) + 2] - e^2 \\ \hat{p}_\varphi &= \hbar[b_1^\dagger b_1 - b_2^\dagger b_2] \\ \hat{p}_{\varphi'} &= \hbar[\tilde{b}_1^\dagger \tilde{b}_1 - \tilde{b}_2^\dagger \tilde{b}_2] \end{aligned} \tag{30}$$

By defining the number operators

$$\begin{aligned} n_k &= b_k^\dagger b_k, \\ \tilde{n}_k &= \tilde{b}_k^\dagger \tilde{b}_k, \quad k = 1, 2 \end{aligned} \tag{31}$$

the total Hamiltonian is given by

$$\begin{aligned} \hat{\tilde{H}}_T &= \hbar\omega[n_1 + n_2 + \tilde{n}_1 + \tilde{n}_2 + 2] - e^2 \\ &= \hbar\omega[2n_1 - \hat{p}_\varphi/\hbar + 2\tilde{n}_2 + \hat{p}_{\varphi'}/\hbar + 2] - e^2 \\ &= 2\hbar\omega[n_1 + \tilde{n}_2 + 1] - e^2 \end{aligned} \tag{32}$$

by noting the physical state condition $\hat{p}_\varphi = \hat{p}_{\varphi'}$.

We thus define the principal quantum number (or its operator) n by

$$n = n_1 + \tilde{n}_2 + 1 = 1, 2, 3, ... \tag{33}$$

and the physical state condition

$$(2n\hbar\omega - e^2)\psi_{phys} = 0 \tag{34}$$

gives rise to the Bohr spectrum

$$E = -\frac{mc^2}{2}(\frac{e^2}{\hbar c})^2\frac{1}{n^2}, \quad n = 1, 2, 3, ... \tag{35}$$

by noting the definition of ω in (7). As for the degeneracy of states with a fixed n, it is confirmed that each state with a given n has n^2 degeneracy.

2.2, Jacobi's Principle of Least Action

The meaning of the total Hamiltonian in (6) becomes transparent , if one starts with a Nambu-Goto-type Lagrangian (the Jacobi's principle of least action for a given E) which is reparametrization invariant,

$$\begin{aligned} S &= \int_0^\tau L d\tau = \int_0^\tau d\tau \sqrt{2m(E - V(r))(\frac{d\vec{x}}{d\tau})^2} \\ &= \int \sqrt{2m(E - V(r))(d\vec{x})^2} \end{aligned} \tag{36}$$

The momenta conjugate to coordinates are then defined by

$$\vec{p} = \frac{\partial L}{\partial \dot{\vec{x}}} = \sqrt{2m(E - V(r))}(\frac{d\vec{x}}{d\tau})/\sqrt{(\frac{d\vec{x}}{d\tau})^2} \tag{37}$$

and one obtains a vanishing Hamiltonian as a result of reparametrization invariance and a first-class constraint ϕ, which is the generator of reparametrization gauge symmetry,

$$\begin{aligned} H &= \vec{p}\dot{\vec{x}} - L = 0 \\ \phi(\vec{x}, \vec{p}) &= \frac{\vec{p}^2}{2m} + V(r) - E \simeq 0 \end{aligned} \tag{38}$$

Following Dirac[19], the total Hamiltonian is defined by

$$\begin{aligned} H_T &= H + \alpha(\vec{x}, \vec{p})\phi(\vec{x}, \vec{p}) \\ &= \alpha(\vec{x}, \vec{p})\phi(\vec{x}, \vec{p}) \simeq 0 \end{aligned} \tag{39}$$

and the function $\alpha(\vec{x}, \vec{p})$ specifies a choice of gauge and fixes the arbitrary parameter τ in (36), which parametrizes the orbit for a given E. A change of the parameter τ to $\tau - \delta\beta(\tau, \vec{x}, \vec{p})$ is generated by $\delta\beta(\tau, \vec{x}, \vec{p})\alpha(\vec{x}, \vec{p})\phi(\vec{x}, \vec{p}) = \delta\beta(\tau, \vec{x}, \vec{p})H_T$, for example,

$$\begin{aligned} \delta\vec{x}(\tau) &= \vec{x}'(\tau) - \vec{x}(\tau) \\ &= \vec{x}(\tau + \delta\beta) - \vec{x}(\tau) \\ &= \{\vec{x}, \delta\beta H_T\}_{PB} \\ &= \delta\beta(\tau, \vec{x}, \vec{p})\frac{d}{d\tau}\vec{x}(\tau) \end{aligned} \tag{40}$$

in terms of the Poisson bracket, since $\vec{x}'(\tau - \delta\beta) = \vec{x}(\tau)$.

Quantization is performed by

$$i\hbar\frac{\partial}{\partial\tau}\psi = \hat{H}_T\psi \tag{41}$$

with a physical state condition

$$\hat{\alpha}(\vec{x}, \vec{p})\hat{\phi}(\vec{x}, \vec{p})\psi_{phy} = 0 \tag{42}$$

A specific choice of the gauge $\alpha(\vec{x},\vec{p}) = r = \xi + \eta$ leads to the Hamiltonian $\hat{H}_T$ in (6) and the choice $\alpha(\vec{x},\vec{p}) = 1$ gives the original static Schroedinger equation(4), since the states ψ in (5) and (4) are physical states. Eq.(41) gives rise to the evolution operator in (11).

We now explain the relations (20)$\sim$(22) in a more concrete manner. We start with eq.(20) for a generic negative E

$$\begin{aligned} G(E;\xi_b,\eta_b,\varphi_b;\xi_a,\eta_a,\varphi_a) &= \langle \xi_b,\eta_b,\varphi_b|\frac{\hbar}{\hat{H}_T(E;\xi,\eta,\varphi)}|\xi_a,\eta_a,\varphi_a\rangle \\ &\equiv \sum_n \phi_n(E;\xi_b,\eta_b,\varphi_b)\frac{\hbar}{\lambda_n(E)}\phi_n^\star(E;\xi_a,\eta_a,\varphi_a) \end{aligned} \tag{43}$$

with

$$\begin{aligned} \hat{H}_T(E;\xi,\eta,\varphi)\phi_n(E;\xi,\eta,\varphi) &= \lambda_n(E)\phi_n(E;\xi,\eta,\varphi) \\ \int \phi_n^\star(E;\xi,\eta,\varphi)\phi_l(E;\xi,\eta,\varphi)dV_0 &= \delta_{n,l} \\ \lambda_n(E) &= 2n\hbar\sqrt{-\frac{E}{2m}} - e^2 \\ dV_0 &= 4\pi \times 2d\xi d\eta d\varphi \end{aligned} \tag{44}$$

where we used the result in (32) and also the variables (ξ,η,φ) instead of (u,v,φ) for notational simplicity. The summation over n in (43) is formal including the n^2 degeneracy. Note that the complete orthonormal states $\{\phi_n\}$ in (43) are all *unphysical* off- shell states. In path integral, the summation in (43) is exactly evaluated in (18).

We next rewrite $G(E;\xi_b,\eta_b,\varphi_b;\xi_a,\eta_a,\varphi_a)$ in terms of physical on-shell states by writing an unsubtracted dispersion relation (i.e., paying attention only to the pole structure in E) as

$$G(E;\xi_b,\eta_b,\varphi_b;\xi_a,\eta_a,\varphi_a) = \sum_n \phi_n(E_n;\xi_b,\eta_b,\varphi_b)\frac{\hbar}{(E_n-E)(-\frac{\partial\lambda_n(E_n)}{\partial E_n})}\phi_n^\star(E_n;\xi_a,\eta_a,\varphi_a) \tag{45}$$

by noting

$$\lambda_n(E) = \lambda_n(E_n) + (E-E_n)\frac{\partial\lambda_n(E_n)}{\partial E_n} = (E-E_n)(\frac{-e^2}{2E_n}) \tag{46}$$

for $E \approx E_n$.

When one defines

$$\psi_n(E_n;\xi,\eta,\varphi) = \frac{1}{\sqrt{-\frac{\partial\lambda_n(E_n)}{\partial E_n}}}\phi_n(E_n;\xi,\eta,\varphi) \tag{47}$$

one can show the orthonormality relations of physical on-shell states

$$\begin{aligned} \int \psi_n^\star(E_n;\xi,\eta,\varphi)\psi_l(E_l;\xi,\eta,\varphi)(\xi+\eta)dV_0 &= \int \psi_n^\star(E_n;\xi,\eta,\varphi)\psi_l(E_l;\xi,\eta,\varphi)dV \\ &= \delta_{n,l} \end{aligned} \tag{48}$$

with $dV = (\xi+\eta)dV_0$. First of all, from the physical state condition

$$\begin{aligned} &\hat{H}_T(E_n;\xi,\eta,\varphi)\phi_n(E_n;\xi,\eta,\varphi) \\ &= \{\frac{1}{2m}(\hat{p}_\xi\xi\hat{p}_\xi + \hat{p}_\eta\eta\hat{p}_\eta) + \frac{1}{8m}(\frac{1}{\xi}+\frac{1}{\eta})\hat{p}_\varphi^2 - E_n(\xi+\eta) - e^2\}\phi_n(E_n;\xi,\eta,\varphi) = 0 \end{aligned} \tag{49}$$

one can establish the orthogonality relation

$$(E_n - E_l) \int \phi_n^\star(E_n;\xi,\eta,\varphi)\phi_l(E_l;\xi,\eta,\varphi)(\xi+\eta)dV_0 = 0 \tag{50}$$

for $n \neq l$. Also from the relation (49) and the fact that the "eigenvalue" e^2 is equally distributed for the kinetic and potential terms for harmonic oscillators(in terms of u and v variables) , we have

$$-E_n \int \phi_n^\star(E_n;\xi,\eta,\varphi)\phi_n(E_n;\xi,\eta,\varphi)(\xi+\eta)dV_0 = \frac{e^2}{2} \tag{51}$$

namely

$$\frac{1}{-\frac{\partial\lambda_n(E_n)}{\partial E_n}} \int \phi_n^\star(E_n;\xi,\eta,\varphi)\phi_n(E_n;\xi,\eta,\varphi)(\xi+\eta)dV_0 = 1 \tag{52}$$

by noting (44). This proves (48).

From (45), we finally arrive at the expression

$$\begin{aligned} G(E;\xi_b,\eta_b,\varphi_b;\xi_a,\eta_a,\varphi_a) &= \sum_n \psi_n(E_n;\xi_b,\eta_b,\varphi_b)\frac{\hbar}{E_n - E}\psi_n^\star(E_n;\xi_a,\eta_a,\varphi_a) \\ &= \langle\xi_b,\eta_b,\varphi_b|\frac{\hbar}{\hat{H}(\xi,\eta,\varphi) - E}|\xi_a,\eta_a,\varphi_a\rangle \\ &= \frac{1}{4\pi}\langle\vec{x}_b|\frac{\hbar}{\hat{\vec{p}}^2/(2m) - e^2/r - E}|\vec{x}_a\rangle \end{aligned} \tag{53}$$

which establishes the gauge independence of the Green's function for negative E. Although we here used the same notation for the state $|\xi,\eta,\varphi\rangle$ in (43) and (53), the meaning of these states are quite different. This difference is explicitly exhibited in (20) $\sim$ (22). It is important to realize that the exact path integral is performed for the off-shell states in (43).

III. CONCLUSION

The path integral treatment of a general separable Hamiltonian of Liouville-type is formulated on the basis of the Jacobi's principle of least action by using a gauge theoretical technique, and it has been illustrated for the hydrogen atom in parabolic coordinates.

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